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Modelling the Fate and Influence of Marine Spray

*Proceedings of a workshop held 6-8 June 1990,
Luminy, Marseille, France*

*Patrice G. Mestayer, Edward C. Monahan,
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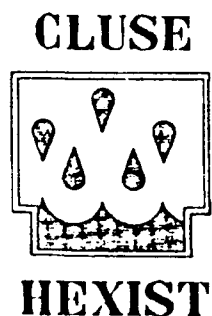
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This workshop brings to a conclusion the international cooperative research program CLUSE - HEXIST 3, 1988-1990, sponsored by the National Science Foundation (via Grant INT-8715148) and the Centre National de la Recherche Scientifique (via Grant AI (06943)8131) under the auspices of the U.S.-France Cooperative Science Program.



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A CONTINUOUS BIN MODEL OF AEROSOL BEHAVIOR IN THE MARINE BOUNDARY LAYER

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The nature of aerosol particles at the ocean surface is important to a large number of direct and indirect applications. Visibility in the optical wavelengths is largely controlled by the distribution of haze particles. The growth of ice and rime on ship structures depends on the concentration of aerosol particles, as well as temperature and water vapor content of the atmosphere. Less directly, aerosols play an important role in the transfer of mass and latent heat from the ocean to the atmosphere. Particularly at high wind speeds, the aerosol population can be responsible for a significant part of the total surface flux of heat and moisture.

Operational Navy applications require a particularly accurate description of the particle size distribution. Since the efficiency of scattering by particles strongly depends on the ratio of incident wavelength and scatterer dimension, visible, infrared, and microwave systems performance are affected by different parts of the aerosol size distribution. In particular, micron droplets attenuate or modify visible imagery, while larger, submillimeter particles affect microwave wavelengths. The microphysics of the aerosol population is therefore important to the development of operational applications.

The behavior of marine aerosols has been studied by several investigators. Ling and Kao (1976), developed a monomodal size distribution model which described aerosol thermodynamics and dynamics in the several meters above the ocean. The assumption has been that the state variables (temperature and humidity) are described by diffusion equations arising from the temperature and humidity gradients respectively. This work has been expanded to other more realistic distributions by Stramska (1986), who has used a discrete bin model of the aerosol size distribution. Burk (1984) has invoked higher order closure to simulate the effect of aerosol behavior on the state variables. This model considered the conservation of marine atmosphere salt particles, which would accommodate to the ambient moisture and temperature. This model

provided the clear advantage that the aerosol growth equations correctly include the solute of a solution on particle growth rates. The detailed dynamics of individual particles has been treated with a Lagrangian model of aerosol transport proposed by Fairall and Edson (1989). The model is currently in use to investigate the anisotropy of aerosol source function around the wave crest.

A common difficulty of these models is the correct description of the detailed vapor condensation and growth on the marine aerosol particles. The microphysics of a droplet population have been successfully described in the context of precipitating clouds by Young (1974). In this model, the aerosol distribution is considered as a piece-wise linear function, modified by the ambient state variables. This model has the advantage of providing a detailed description of the aerosol size distribution, as well as being somewhat more realistic in the treatment of condensation, evaporation, and coagulation in precipitating clouds. The following paper applies the piece-wise continuous aerosol model to the behavior of marine aerosols near the ocean surface. The marine atmosphere is considered as three connected systems: state variables, continuous aerosol processes, and discrete aerosol processes. The state variables of temperature and moisture behave according to the accepted first order closure (K theory) assumptions. The continuous aerosol processes consist of evaporation and condensation. The discrete processes involve the changes of numbers particles either by motion to an adjacent layer, or by injection of aerosols from wave breaking or other mechanisms at the surface. The model provides a description of the vertical distribution of aerosols in the turbulent boundary layer within 100 m of the ocean.

Governing Model of the Atmospheric Surface Layer

Our model describes the near surface marine atmosphere by a vertical logarithmic grid. At each grid point we maintain the values of temperature humidity, and aerosol parameters. Aerosol parameters considered by the model are the number and mass of aerosol particles in groups defined by a smallest and largest radius. The aerosol parameters are modified by a continuous change model which describes the vapor condensation onto and the evaporation from the particle surface, and the discrete change model which considers particle vertical motion and injection from the surface.

State Variables in the Atmospheric Surface Layer

The temperature and humidity behavior of the atmosphere within 100 m of the ocean surface have been successfully described with the assumption of a constant flux layer. The state variables, potential temperature and specific humidity, obey the standard diffusion equation (Businger, 1973), perhaps with a source term accounting for the moisture and temperature change due to injected or falling aerosols within an air parcel. Strictly speaking, the conservative temperature variable is potential temperature, but within the first hundred meters above the ocean surface, the difference between potential temperature and the temperature is negligible. Henceforth temperature will be considered as the conservative heat variable.

The conservation equation for the state variable X is

$$\frac{\partial X}{\partial t} = \frac{\partial}{\partial z} \left[K_z \left(\frac{\partial X}{\partial z} \right) \right] + S_x \quad (1)$$



where t is time, z is the vertical coordinate, K_x is the diffusion coefficient for state variable X , and S_x is the source function. In this case the source function is the latent heat of water evaporating or condensing for temperature, and the specific humidity for moisture.

Aerosol Moisture Source Function

The atmospheric moisture source consists of the water vapor by the evaporating drop. The amount of mass evaporated from the drop is provided by Pruppacher and Klett (1976) as

$$\frac{dm}{dt} = 4\pi C D_v (\rho_\infty - \rho_{sat}(r)) \quad (2)$$

where m is condensed mass in gm, C is a growth and ventilation constant, D_v is the diffusivity of water vapor ($\text{cm}^2 \text{sec}^{-1}$), ρ_∞ is the ambient specific humidity in the region of the particle, and $\rho_{sat}(r)$ is the saturation specific humidity at the surface of an aerosol of radius r .

The saturation vapor pressure over a droplet of size $\rho_{sat}(r)$ is given by the Koehler equations (Pruppacher and Klett, 1978),

$$\frac{\rho_{sat}(r)}{\rho_{sat}(\infty)} = 1 + \frac{A}{r} - \frac{B}{r^3} \quad (3)$$

$$A = \frac{000033}{T} B, = \frac{4.3vm_s}{M_s} \quad (4)$$

where v is the van't Hoff factor, m_s is the mass of salt in the droplet, and M_s is the gram molecular weight of salt. The Koehler equation is evaluated with units of radius in cm, temperature T in Kelvin, and mass in grams. The second term is responsible for the effect of solute on evaporation. In this work we consider the solutes shown in Table 1. The solutes are

Table 1. Chemical constants of salts in sea water.

Salt	van't Hoff Factor	Molecular Weight
NaCl	2	58.454
NaNO ₃	2	85.005
(NH ₄) ₂ SO ₄	3	132.146

considered to have a uniform mass of 10^{-15} gm. This was chosen for future consideration of smaller particles, since we found the solute effects to be negligible except for particles smaller than 10^{-4} cm in radius. Testing is being done on the effects of different compositions on the particle growth in the context of this modeling effort.

Temperature

The temperature change of the system is attributed to the flux gradient of temperature and a source from the latent heat absorbed or released by the aerosol particles within a parcel. The general equation (1) becomes

$$\frac{\delta T}{\delta t} = \frac{\delta}{\delta z} \left(K_H \frac{\delta T}{\delta z} \right) + L_s \frac{dm}{dt} \quad (5)$$

where the latent heat of evaporation of water is given by (Pruppacher and Klett, 1978) as

$$L_s = 597.3 \left(273.15 \frac{1}{T} \right)^2 y = 0.167 + .000367 \cdot T. \quad (6)$$

The Marine Aerosol Model

The aerosol population varies because of local condensation and evaporation, gravitational deposition, turbulent transfer, and injection from the wave covered surface. The processes can be separated into continuous processes, in which mass is considered to change continuously, and discrete processes, in which the aerosol number is changed by injection or dynamic motions. The continuous processes are considered by using the change of a piecewise continuous function; discrete processes are described with a conventional gridded bin structure.

The particle population is separated into a number P of adjacent bins. Within each bin the number density is assumed to vary linearly with radius. The particle number distributions are then given by,

$$n_r = n_{r_0} + k_{r_0} (r - r_0), \quad (7)$$

where r_i is the mid point of the radius bin, and n_{r_0}, k_{r_0} are determined from the aerosol distribution observable parameters.

The number concentration of particles in an air parcel with sizes between the limits of a bin is given by.

$$\begin{aligned}
 N &= \int_{r_1}^{r_2} n_r dr \\
 &= (n_{r,\rho} - k_{r,\rho} r_1) R_1 + k_{r,\rho} R_2.
 \end{aligned}
 \tag{8}$$

where we use the shorthand notation,

$$R_n = \frac{(r_2^n - r_1^n)}{n}$$

The total mass within a size bin is given by

$$\begin{aligned}
 M &= \int_{r_1}^{r_2} \left(\frac{4\pi}{3} \right) \rho_r r^3 n_r dr \\
 &= \frac{4\pi}{3} \rho_r [R_4(n_{r,\rho} - k_{r,\rho} r_1) + k_{r,\rho} R_5].
 \end{aligned}
 \tag{9}$$

The number and mass equations can be solved for the distribution parameters with the result

$$\begin{aligned}
 n_{r,\rho} &= \frac{N}{R_1} \\
 k_{r,\rho} &= \frac{\frac{3M}{4\pi\rho} - R_4 N}{r_1 R_1 R_4 - R_1 R_5}
 \end{aligned}
 \tag{10}$$

Continuous Transfer of Aerosols - Evaporation and Condensation

The change in dimension resulting from the additions of mass is given by

$$r_x = \left[r_2^3 - \left(\frac{\Delta M}{N} \right) \frac{3\pi\rho}{4} \right]^{1/3} \tag{11}$$

where the assumption is made that the change in mass is distributed uniformly over all particles. Following this change in mass, the number of particles transferred to another bin consists of those particles which have grown (shrunk) to a size larger (smaller) than the current bin limits. The number of particles growing to the next larger size is given by

$$\delta N = \int_{r_1}^{r_2} n_r dr \quad (12)$$

Discrete Transfer of Aerosols Sedimentation

The sedimentation of particles within a layer was calculated assuming a uniform fall speed within each size bin. Droplet fall speeds were calculated using the fall speed of a particle of radius equal to the mean particle radius in the bin. The fall speed was the unmodified Stokes fall speed,

$$v = \frac{2ga}{9\nu} \quad (13)$$

The change in the number of particles in the bin is given by

$$\Delta N_i^n = N_i^n F_i - N_{i+1}^n F_{i+1} \quad (14)$$

where N are the particle number concentrations, and F are fractions of particles lost or gained by sedimentation. The fraction of particles leaving a layer during a time interval is

$$F_{i+1} = \frac{v \Delta T}{\Delta z} \quad (15)$$

The time interval and mean size must be chosen judiciously so that particles do not uniformly fall through their air parcels.

Injection

The aerosol source function is considered to be an actively breaking wave, providing an aerosol source injecting particles with a range of upward vertical velocities. Rather than an Eulerian scheme tracking each particle, we model the phenomena with an injection function which is height dependent. The source function at the surface is the source function of Marks and Monahan (1988). This function is translated to the parameters of a modified Gamma, or Nukiyama-Tanasawa distribution, using a maximum likelihood method for choice of parameters.

(Goroch, 1980). This function is dependent on wind speed with a power law dependence, following observations of Monahan et al. (1983). The vertical distribution is exponential, to reproduce observations of DeLeeuw (1986).

Initial Conditions

The initial conditions of the model were calculated assuming a well mixed atmospheric surface layer, defined by the 10m value of temperature, specific humidity and wind speed. The vertical profiles of these were initially calculated using Monin-Obukhov scaling as reviewed by Smith (1989). The three relevant equations for wind speed, specific humidity and potential temperature are, respectively:

$$u(z) = \frac{u_*}{k} \left[\ln \left(\frac{z}{z_o} \right) + \psi_u \left(\frac{Z}{L} \right) \right] \quad (16)$$

$$q(z) = \frac{q_*}{k} \left[\ln \left(\frac{z}{z_o} \right) + \psi_q \left(\frac{Z}{L} \right) \right] \quad (17)$$

$$\theta(z) = \frac{\theta_*}{k} \left[\ln \left(\frac{z}{z_o} \right) + \psi_\theta \left(\frac{Z}{L} \right) \right] \quad (18)$$

The flux quantities were obtained from the initial conditions by using the flux profile calculations of Smith (1988).

Summary

This model of the aerosol dynamics in the marine boundary layer emphasizes the microphysics of particles in the marine boundary layer. The several processes affecting the motion and growth of particles are separated into larger scale changes of the temperature and moisture, and the discrete and continuous change of the aerosol number and mass distributions. The method is applied to a Lagrangian model, but could as well be applied to an Eulerian description of aerosol dynamics.

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